

Computational modelling of an aerosol extraction device for use in COVID-19 surgical tracheotomy

Hadrien Calmet^a, Pablo Ferrer Bertomeu^b, Charlotte McIntyre^b, Catherine Rennie^b, Kevin Gouder^b, G. Houzeaux^a, Christian Fletcher^c, Robert Still^c, D.J. Doorly^b

^a*Barcelona Supercomputing Center (BSC-CNS), Department of Computer Applications in Science and Engineering, Edificio NEXUS I, Gran Capitán 2-4, 08034 Barcelona, Spain*

^b*Imperial College London, Department of Aeronautics, Exhibition Road, London SW7 2AZ, UK*

^c*Mercedes-AMG Petronas Formula One Team, Brackley, Northamptonshire, UK*

Abstract

In view of the ongoing COVID-19 pandemic and its effects on global health, understanding and accurately modelling the propagation of human biological aerosols has become crucial. Worldwide, health professionals have been one of the most affected demographics, representing approximately 20% of all cases in Spain, 10% in Italy and 4% in China and US. Methods to contain and remove potentially infected aerosols during Aerosol Generating Procedures (AGPs) near source offer advantages in reducing the contamination of protective clothing and the surrounding theatre equipment and space. In this work we describe the application of computational fluid dynamics in assessing the performance of a prototype extraction hood as a means to contain a high speed aerosol jet. Whilst the particular prototype device is intended to be used during tracheotomies, which are increasingly common in the wake of COVID-19, the underlying physics can be adapted to design similar machines for other AGPs. Computational modelling aspect of this study was largely carried out by Barcelona Supercomputing Center using the high performance computational mechanics code Alya. Based on the high fidelity LES coupled with Lagrangian frameworks the results demonstrate high containment efficiency of generated particles is feasible with achievable air extraction rates.

Keywords: CFD, round turbulent jet, LES, bioaerosols, COVID-19

1. Introduction

Healthcare workers are facing severe challenges to protect themselves effectively from COVID-19. Global scarcity of protective equipment, together with limited initial understanding of the virus and lack of testing capacity translated to many professionals being infected (bbc, 2020). In the first months of 2020, healthcare workers represented 20% of all cases in Spain, 10% in Italy and 4% in China and US (elp, 2020). A few months ago, the International Council of Nurses (ICN) estimated that healthcare worker COVID-19 fatalities worldwide could be more than 20,000 (icn, 2020). A number of surgical and medical procedures have been classified as Aerosol Generating Procedures (AGPs) and there is naturally great interest both in quantifying the aerosol generated in such procedures and in designing engineering controls to better protect healthcare workers. One such procedure is tracheotomy. Briefly, a tracheotomy is the creation of an opening (stoma) in the trachea to the exterior, facilitating ventilation. Strictly tracheostomy refers to the created opening and tracheotomy to the procedure, but the terms are often interchanged. Tracheotomies are performed on approximately 10% of all COVID-19 Intensive Care Unit (ICU) admissions in the UK. Hence, according to this data, tracheotomies are executed in around 1% of the total confirmed cases of COVID-19 (National Tracheostomy Safety Project. Multidisciplinary COVID-19 tracheostomy guidance).

Airborne diseases are those that are spread through the air by small particles. These include tuberculosis, influenza and coronavirus. Tuberculosis is caused by bacteria, while influenza and coronavirus are viruses; however, they share similar mechanics of propagation. Pathogens are spread from infected individuals through bioaerosols, generated in increasing quantities by breathing, talking, coughing and sneezing. Aerosols of the order of $1\ \mu\text{m}$ can remain suspended for hours and, in the absence of data, are assumed to remain infectious for equally long periods. When coughing, some of the surfactant and infected epithelial cells might be pulled from the lungs and into the environment (Mason,

2020). These might also mix with the mucus in the trachea and saliva in the mouth, making them infectious as well. In a study of SARS and H1N1 influenza (Robinson et al. 2011), state that “small droplets ($\approx 0.4\mu m$) generate a negligible infectious force due to the small viral load and the associated duration they require to transmit infection. In contrast, larger droplets ($\approx 4\mu m$) can lead to an infectious wave propagating through a fully susceptible population or a secondary infection outbreak for a localised susceptible population” (Robinson et al., 2012). As yet we cannot quantify the relative importance of parameters such as aerosol size, concentration and exposure time in terms of risk of infection, all of which depend on the strain of virus and the particular context. The context of interest here is with minimising short time exposure of health care staff to airborne particles in tracheotomy and similar procedures.

A few measurements of particle generation during tracheal procedures are now available, including Brown et al. (2021), Dhillon et al. (2020) on aerosol generation during tracheal intubation/extubation procedures. These were each small studies on non-Covid-19 patients. Both reported elevated aerosol generation during intubation and extubation. Brown et al reported lower aerosol generation in extubation than in a volitional cough, though caution that their study did not include patients with respiratory comorbidities. Depending on the level of sedation, coughing can also be associated with extubation. Aerosol generation was also found to occur during various phases of a percutaneous tracheotomy procedure in a single uncomplicated case, Ramesh et al. (2020), in which lower aerosol production was recorded than in a cough. However in a case report of a surgical tracheotomy on a SARS-Cov2-positive patient, McGain et al. (2020), inadvertent bronchial intubation led to a very large increase in particle release, which the authors suspected as due to an increased airway pressure surpassing the endotracheal tube cuff pressure. Moreover as described in O’Mahony & Martin (2020), procedures such as moving from endotracheal tube to tracheostomy has potential for aerosol generation, while change or removal of tracheostomy involves suctioning, triggering forceful coughing.

This paper is organized as follows. Section 2 presents the design requirements

used in this study, Section 3 describes the test case, Section 4 presents the construction and tests performed for the prototype, then Section 5 exposes the computational model used following by the results (Section 6 and 7) while the conclusion is presented in Section 8.

2. Design requirements

With this outlook, the NHS reached out to Imperial College to investigate if a device could be designed to reduce the risk of infection during AGPs. The device should be proven to work under the worst-case scenarios, should be simple to manufacture and reasonably economical. There have already been a number of AGP protective devices, which aim to limit the spread of aerosols and droplets from a patient undergoing procedures such as extubation. Broadly these can be classified as methods relying on a physical barrier (e.g. as simple as plastic sheeting Matava et al. (2020b) or rigid boxes), methods using enclosures combined with a degree of suction, (e.g. as described by Perella et al. (2021), Phu et al. (2020)), and methods which may include some shield or barrier, but which primarily rely on capture of aerosol by suction. An example of the latter is described in the model study reported by Matava et al. (2020a), in which the capture performance is studied for a conical nozzle placed 25 - 35 cm above the mouth of a mannikin.

However whereas enclosures have been used for intubation/extubation, they restrict movement. For a surgical procedure such as tracheotomy, as near as possible unhindered access was deemed essential by the surgical team and hence enclosures, though highly effective, were ruled out. Attention therefore focussed on the design of a shield device with powerful extraction.

When designing a medical device, it is also important to ensure compatibility with as many patients as possible. In the case of COVID-19, this is difficult because the range goes from the elderly (low body mass index (BMI), short) to adult overweight male patients (high BMI, tall). This means the device needs to adapt to the patient and have a certain degree of flexibility or it needs to

be designed for one extreme case scenario and proved to work for the other. In terms of the patient position, tracheotomies are carried out with the patient lying supine (face up) on an operating table, with very limited movement (highly sedated). The table's height can be adjusted to the surgeon's preference. The machine should not interfere with the surgeons and should be optically clear to allow good visibility. Hence an open hood structure of transparent material was selected in contrast to a closed portable hood as described in Phu et al. (2020) or Perella et al. (2021).

During a tracheostomy there can be several healthcare workers around the patient. This limits the size of the designed shield or hood to approximately the size of the operating table, since it will disturb the surgical team if it extends further. Other constraints exist for the piping, but those are not relevant to the simulations. In terms of suction, it would be ideal to minimise it while guaranteeing safety. Low power suction pumps are generally cheaper and more readily available since they can be sourced from commercial vacuum cleaners. Furthermore, lower suction vacuum pumps are normally quieter and possibly easier to filter, as they require smaller filters. Having decided on the geometrical constraints for the device, the next stage is to devise appropriate tests for prototypes.

3. Test scenario

Clearly there exist multiple different AGP processes, depending on the patient and the operating procedure under consideration. For the tracheotomy procedure, the patient is sedated and the surgical team is primarily concerned with the possibility of a jet of flow escaping from the tracheostomy site. Based on surgeon's suggestions, the test case considered a high speed jet escaping through a small opening of the trachea. It was decided to perform high resolution computations considering only one unsteady jet flow rate with a simplified on/off temporal profile. Given a suitably energetic jet, this should meet the twin objectives of both investigating the performance of the device and pro-

viding accurate data to check lower resolution simulations of this and future devices. Though not considered here, the present study may be relevant to the post-operative tracheostomy care, since cleaning and changing the tracheostomy often provokes coughing, also of concern as an AGP.

During a tracheotomy, it is recommended that the ventilator is turned off while the trachea is opened, but time off ventilation needs to be minimised so the lungs may remain pressurised. Furthermore, during initial creation of the tracheotomy, ventilation is maintained via endotracheal tube. Usually the presence of an inflatable cuff seal would prevent escape from the patient airways to the exterior, but the quality of the seal has to balance inflation pressure against the possibility of damage to the trachea. There is also the possibility of failure of the seal, with ventilation continued momentarily. In the worst case, the lungs could be pressurised to a delivery pressure of 10 - 15 cm H₂O or approximately 1 - 1.5 *kPa*, providing sufficient reservoir pressure to accelerate an aerosol jet from the trachea to the surroundings.

One of the difficult aspects of the simulation is deciding on the incision size. Since the lungs are a pressurised environment, the smaller the incision, the faster the jet of flow generated (until choking of the flow, which is anyway impossible). The selected case was the circular opening due to correspond with that for cannula insertion. Based on the report “how design characteristics of tracheostomy tubes affect the cannula and tracheal flows” (Subramaniam et al., 2019), the diameter was selected for 4.7 mm (diameter of an outer cannula tube) and 2.7 mm internal diameter. Assuming negligible pressure loss for flow accelerating through such a narrow tracheal opening, a pressure maintained at the above level would induce a flow of 0.27 - 0.33 $l.s^{-1}$ or 16 to 20 $l.min^{-1}$. Assuming a flow duration of 2 seconds at a flow rate of 0.3 $l.s^{-1}$ provides a total volume of 0.6 *l*.

The total expired volume (at approximately 0.7 *l*) for such a tracheal jet compares reasonably with that of cough generated flows through the mouth according to Gupta et al. (2009), range (0.4-1.6 *l*), though is lower than that in other studies reported by Gupta et al. (2009). However the exit velocity

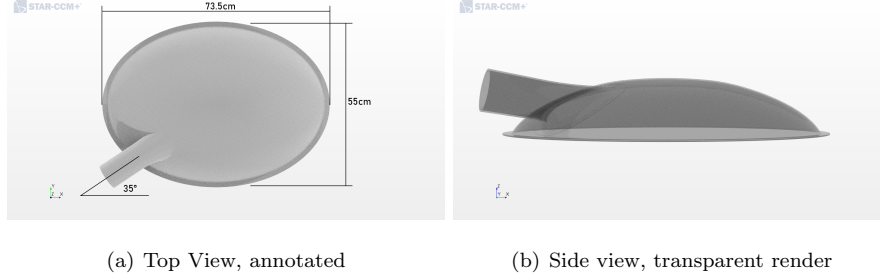


Figure 1: Prototype suction hood renders

for this tracheal jet, at 55 m.s^{-1} is considerably greater than the $6 - 22 \text{ m.s}^{-1}$ range referred to in Gupta et al. (2009); combined with the virtual instantaneous acceleration to full flow, a more intense initial vortex is expected to occur for the flow considered in this study. It was therefore decided that this flow simulation would provide a suitable containment test.

4. Prototype construction and testing

Based on the initial simulations and after consulting NHS professionals, the Mercedes F1 Team manufactured an initial prototype of the proposed machine. This prototype was 55 cm by 73.5 cm (due to size constraints explained above). Preliminary CFD showed flexible skirts greatly enhanced containment efficiency, and suction directly above the incision was most effective. Both of these were ruled out by surgeons as they would impede access and vision respectively. The suction pipe was therefore thought the side instead of the top, see Fig.1. This device is referred as the Mk 1 in this study. Finally, note that the extraction pipe is inclined 10° from the horizontal plane and has a diameter of 8 cm.

Some wind tunnel testing using smoke particle visualisation (Seeding Generator Model 9010F0031, Dantec Dynamics, 1:4 polyethylene glycol:water, particle size range $1 - 3 \mu\text{m}$) was carried out with the Mk 1 suction hood at different suction rates and different angles (from 0 to 20 degrees to the horizontal), see Fig. 2. High speed cameras were deployed, and several experiments were carefully captured and logged. Within the small range of angles, suction rate

appeared dominant and was the main focus of experimental tests. Some leakage was spotted at the low suction rates (46 l s^{-1}) shown in Fig. 2, but none at higher extraction rates (77 l s^{-1}), used for the subsequent simulations.

Using the Mk 1 geometry files provided by Mercedes, a few preliminary simulations were ran to check the visual similarity between experiment and CFD results, i.e. how closely the computed aerosol plume behaviour matched that observed in testing.

Initially, a large difference was found in terms of leakage and overall flow behaviour. After some further testing, it became clear that the problem with the simulation was that both the applied suction and the flow jet from the cannula commenced at the same time. If the jet is started too early, it escapes the hood before the suction flow has become fully established. Since the Mk 1 hood is large and has a long extraction pipe, the velocity field would take a time to settle (estimated as long as the volume below the hood divided by the suction rate, i.e. of order 2 - 3 seconds). However, in the experiment, suction was started before allowing the aerosol jet to escape, representing a sensible scenario for actual operation, where suction would be turned on before creating the tracheostomy.

Therefore a more realistic simulation was prepared. It would run a steady state simulation with just hood suction until convergence, defining the initial boundary condition for the time-dependent computation. With the suctioning velocity field thus established, the transitional inflow jet was then switched on, matching the operation of the experiment.

In terms of the values used for this simulation, the extraction fan was experimentally measured to extract 77 l s^{-1} of ambient air. The inlet cannula was measured to input 0.3 l s^{-1} , corresponding to 0.3675 g s^{-1} neglecting the effect of smoke on the density. The inlet into the domain was a small pipe with an internal diameter of 2.7 mm and an outer diameter of 4.7 mm. All the informations related to the cannula are validated by the surgeons.

A fast simulation was run to check the geometry and velocity flow rates, but the focus quickly shifted towards high fidelity simulations, which can capture

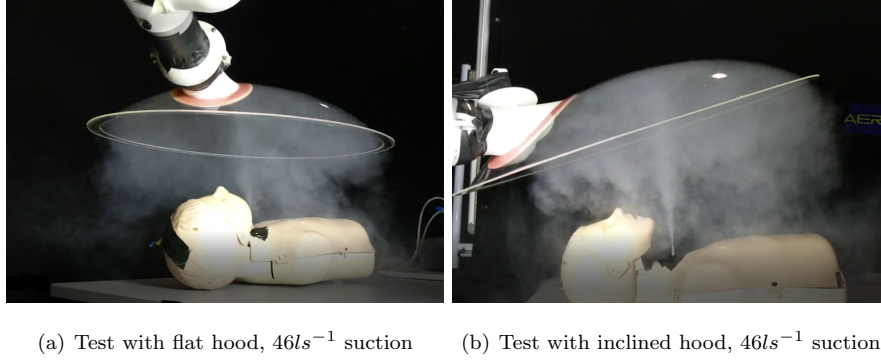


Figure 2: Prototype suction hood in wind tunnel tests

the intermittency of the turbulent jet flow much more accurately. Thanks to the Barcelona supercomputing center this aspect can be considered: running this simulation on a supercomputer allows for both a fine mesh and low timestep, greatly reducing the amount of artificial diffusion and improving the accuracy of the simulation.

5. Computational model

5.1. Mesh generation

The computational model (see Fig. 3) was used to generate a high resolution unstructured mesh with ANSYS ICEM CFD (ANSYS Inc., USA). A first refinement zone set to 1 mm element size was created to capture the features of the jet, then another refinement zone around the jet as a hood extension set to 5mm (see Fig. 3). The Delaunay method was used to provide a smooth cell transition ratio (~ 1.2) between the different sized refinement zones. More details concerning the mesh of the hood surface and that within the hood are available in the appendix section, see Fig. 12. Different meshes were used in this study; medium one (M1) with 5 million tetrahedral elements was used to set and check the parameters of the simulation, although the fine mesh M2 contained 9 million tetrahedral elements and was used to perform all the results presented in the study. Furthermore, M2 found a good balance between

computational costs and solution accuracy reaching a ratio between the grid size and the smallest scales of turbulent motions equal to 8, which satisfies the criterion of sufficient grid resolution for LES. Moreover the time resolution of the LES simulation was sufficiently small to capture the highest frequencies of turbulence. All the information about the grid convergence test are available in the appendix section.

5.2. Computational aspect

As described in the previous section, observing the dynamic aspect of this aerosol transmission was a key aspect of this simulation, with a fine mesh and low timestep being the requirement to capture the unsteadiness. The computational mechanics code Alya (Vázquez et al., 2016), developed at Barcelona Supercomputing Center (BSC) was used, to model the Navier-Stokes equation. For the high fidelity LES simulation, an eddy-viscosity subgrid-scale model (Vreman model) (Vreman, 2004) was applied. Details of the model and parameters used in the simulations are given in Table 1 and the appendix section. With the use of supercomputer Marenostrum hosted by BSC, the simulation time was greatly accelerated, so that only 60 hours running on 480 cores were needed to resolve a 5 second simulation.

5.3. Boundary conditions

To test the efficiency of the suction under realistic conditions an unsteady inflow jet and an initial flow field were applied. The boundary conditions used in this simulation are detailed in Sec.4. Clearly there exists multiple different jet conditions, greatly depending on the patient. In the present study we used only one jet flow rate based on surgeon remark with a simplified profile for the unsteady aspect. The unsteady jet of air coming out of an opening was modeled with $55m/s$ which correspond to $0.3ls^{-1}$ during $2s$ and the internal cannula diameter (D) was $2.7mm$. The initial flow field was set to establish the flow pattern of the hood suction even before the jet begins; this means that a pre-simulation was needed to initialize the velocity and pressure fields.

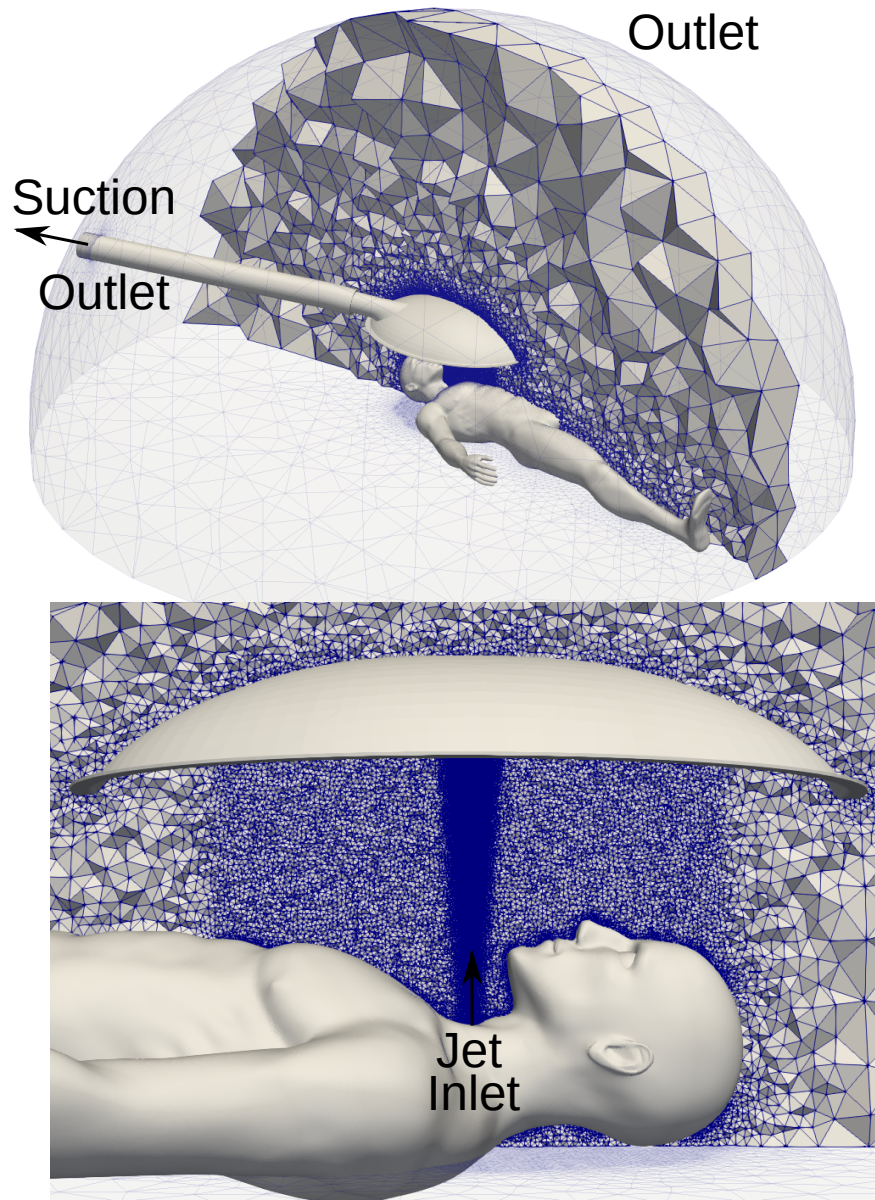


Figure 3: Mesh generation with general view on the top and different mesh resolution in selected slice on the bottom.

Mesh	Model	Δt Algorithm	N_{CPU}	$\Delta t(s)$	CPU/ite (s)	N_{ite}	time (h)
M2	LES	Explicit(RK4)	480	$1.09e^{-5}$	0.2	786372	60

Table 1: Summary of different parameters with Model: turbulence model, Δt Algorithm: time step strategy, N_{CPU} : number of CPU, Δt : time step, CPU/ite: elapsed time per iteration, N_{ite} : number of iterations and time: total time of the simulation(5s).

The Dirichlet condition was imposed as inflow velocity at the jet inlet of the cannula and the suction outlet velocity at the end of the suction pipe. The former condition was imposed to mimic the suction flow rate equivalent to $77L/s$. A zero-traction outflow condition was imposed at the hemispherical surface as a Neumann condition (the surface is free from external stress), see Fig 3. The rest of the surfaces are treated as a no-slip boundary condition. The outer hemisphere is large enough to ensure that the flow induced by the jet and suction are reduced to negligible values at the outer boundary, thereby ensuring that the outlet boundary condition does not affect the flow field.

6. Results: Jet features

The jet generated by a tracheostomy flows into an ambient air of the same fluid, which is not at rest at infinity. As explained below the suction and the presence of the shield at $0.34m$ ($125D$) of the nozzle affects the surrounding jet. The flat-topped velocity profile at the nozzle is $U_j = 55m/s$ and the diameter of the inlet orifice is $D = 2.7mm$. The Reynold number based on the diameter is $Re_d = 8000$. From Pope (Pope, 2000) the jet regions can be divided into 2 parts; the developing region ($< 30D$) and the self-similarity region ($> 30D$) where universal values are observed as angle or profile of velocity variables. The universal angle of penetration is 11.8° which is not the value that we observed, see Fig 4. The mean radial and axial velocities are averaged after the jet is fully developed during $0.4s$, every $0.05s$, means 8 averaged periods which are averaged. $0.05s$ come from 1000 times T_τ ($T_\tau = d/U_j$).

Some profiles are plotted in Fig.5 beyond the developing region ($x/d > 30$,

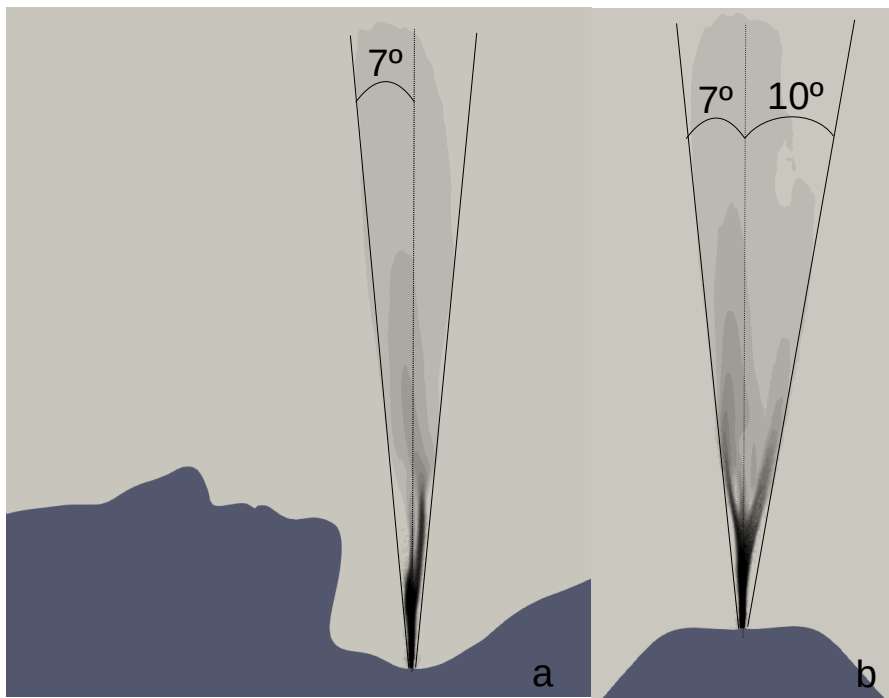


Figure 4: Jet penetration through mean velocity in (a) sagittal and (b) transversal view.

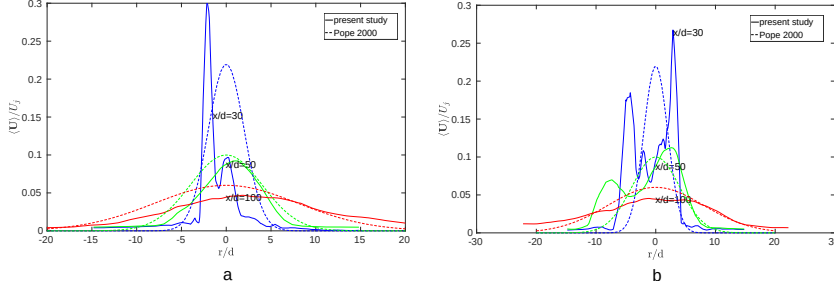


Figure 5: Radial profiles (a) sagittal and (b) transversal slice of mean axial velocity

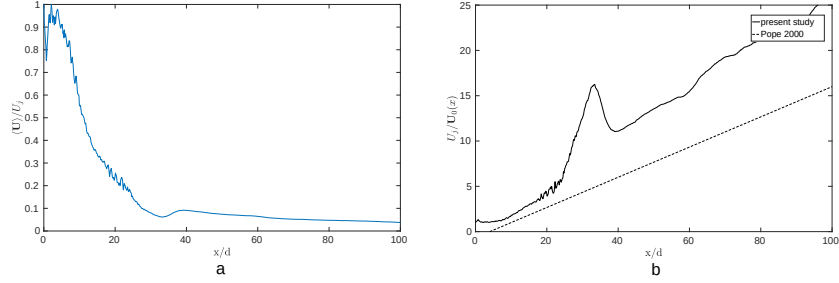


Figure 6: (a) mean axial velocity versus radial distance and (b) the variation of the maximum velocity of the jet versus distance along the axis jet

say). The jet is non axisymmetric. The dashed lines are from the data of Pope (Pope, 2000).

Following the jet analysis on the self-similarity region, Fig 6(a) shows the mean axial velocity versus radial distance. The velocity is scaled by the flat-topped velocity profile at the nozzle, referred to as U_j . Then Fig 6(b) shows the variation of the maximum velocity of the jet versus distance along with the axis jet.

Referring back to the non-axisymmetric nature of this jet, Figures 4,5, different considerations may explain this asymmetry. The first one is the location of the nozzle. In fact, on the left and right side of the neck, the air is free to flow towards the jet and to be entrained without obstacle, which is not the case for air above and beyond the neck, because of the presences of the head and chest.

Thus, this creates an imbalanced configuration of ambient air flowing into the jet. Other reasons are the initial condition exposed previously and the effects of the suction, expected to reduce the angle of the jet. All of these facts made comparison with the jet literature and the jet analytical solution impossible.

7. Particle results

The incision for the tracheotomy produces the release of the bio aerosols in the surgery room; the injector is located on the circle surface of the cannula where particles are distributed uniformly. In this study a simplified model of uniform particle distribution is used. Based on (Robinson et al., 2012; Anand & Mayya, 2020; Johnson et al., 2011) four different sizes are injected, 1, 10, 30 and 100 μm to cover the likely range of emitted particle sizes, from those that move with the flow to those where the ballistic component is of growing magnitude. They are initially released at the beginning of the jet period and reinjected every 1 ms until the end of the jet (2s). 50000 particles for each type are released in the domain to ensure constant deposition value independent of the number of injected particles. No change in deposition proportions was found for particle numbers exceeding 17000, even for the smallest and most sensitive type. The initial velocities of the particles are assumed to be the same as the inflow velocity at the entrance of the cannula. The total time of the simulation is 5s to observe the total suction of the aerosols from the hood extractor, see Fig.7 (which is a screenshot of the animation available in the supplementary material). It is observed from the animation that almost all the particles are deposited or out of the extractor after 5s. A deeper analysis is now carried out to accurately quantify the fate of the bioaerosols. All the aspects of the particle transport equations and deposition modeling are exposed in the appendix section.

The dynamics of the particles are different as a function of the diameter and thus the deposition location; if the particle settles or it is sucked through the extractor. Table 2 and Fig.8 show the fate of the particles released during the incision for the tracheotomy. Following individual particles provide information

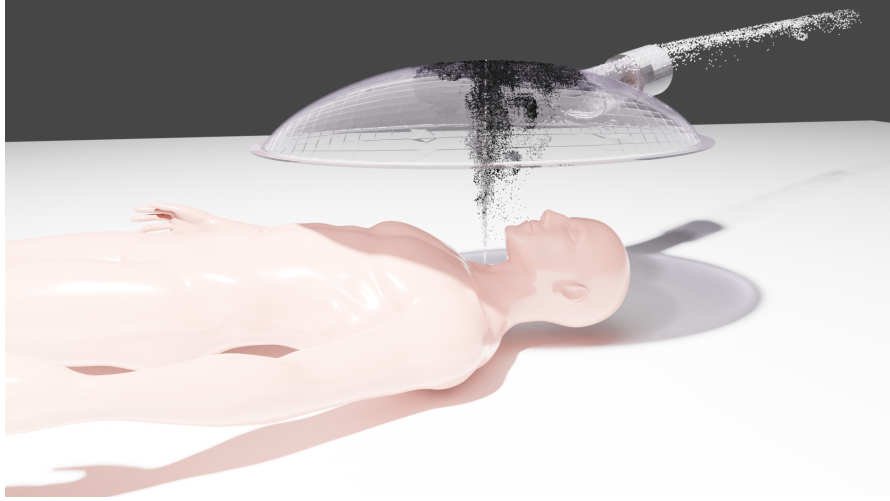


Figure 7: Screenshot of the animation available in the supplementary material

of trajectory, for example; if they cross the virtual boundary located from the edge of the shield extractor, up to the patient, we can evaluate the efficiency of the extractor.

Fig.9 shows some trajectories for each type of particle diameter. As expected the largest particles ($100\ \mu m$, blue color) with higher inertia are almost all deposited in the shield with 99.6% of deposition due to the deviation of the particle paths, see Fig.8. The medium-sized particles (10 and $30\ \mu m$, white and red colors, respectively) are mainly sucked out of the computational domain through the extractor; due to the smaller inertia, the particles mostly followed the streamlines of the flow and a very low percentage of the particles remain still floating in the room. The most important mechanism of deposition for the 10 , 30 , and $100\ \mu m$ are the inertial impaction. Now concerning the deposition for the smallest particle size ($1\ \mu m$, black color) this is less straightforward since it is a mix of deposition mechanism: the inertial impaction and the turbulence dispersion occurring during the jet. The latter produces a shear layer on the boundary of the jet core which favors the dispersion of the smallest particles due to the turbulence. It is well known that the vortical structures called the rings

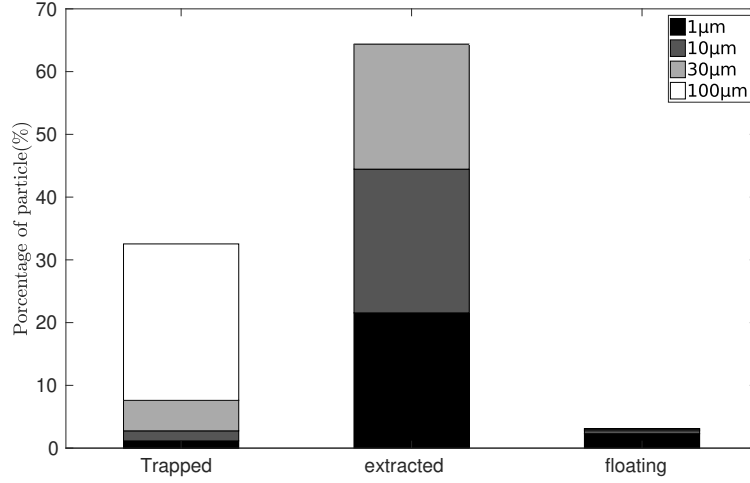


Figure 8: particle deposition represented in bar percentage

of the jet will create clusters of particles which in this case are the smallest. These structures enhance the dispersion of the smallest particles in the near vicinity of the jet as only 0.014% of $1\ \mu m$ particles cross the virtual curtain of the extended shield extractor and 9.2 % are still floating in the room. Those trajectories are not shown in Fig.9.

This study proves that the extractor is an effective way in avoiding extensive contamination in the operating theatre.

8. Conclusion

The purpose of this study was to evaluate the performance of an open hood extraction device to reduce the risk of infection during an AGP. The specific interest was to explore numerically the dynamic aspect of a narrow, high speed transient jet flow issuing from a tracheotomy site and to be able to track the bioaerosols released into the operating room. There are limitations in the scope of the study performed and the modelling used, for example the neglect of aerosol particle shrinkage due to evaporation, and the focus on a single condition. These

Diameter	η_{shield}	Extracted	Crossing	still floating
1 μm	4.6	86.1	0.014	9.2
10 μm	6.4	91.5	0.009	1.9
30 μm	19.4	79.5	0.003	1
100 μm	99.6	0.026	0	0.3

Table 2: Results of particle deposition represented in percentage, with η_{shield} deposited particle on the shield and the body. Extracted: particles going out of the computational domain through the extractor. Crossing: particles crossing the virtual curtain located to the extended shield. Still floating: particles still in the computational domain after 5s of simulation.

are areas for further work. However thanks to a novel machine designed in a collaboration between Mercedes AMG F1 Team and Imperial College London and the computational effort from Barcelona Supercomputing center the simulations demonstrate the efficiency of shield-augmented suction as an aerosol extraction device for use in surgical tracheotomy. This type of device offers advantages in reducing significantly the contamination of protective clothing and the surrounding theatre equipment and space, whilst allowing good access and freedom of movement for the surgical team; it may also be of relevance to other surgical operations.

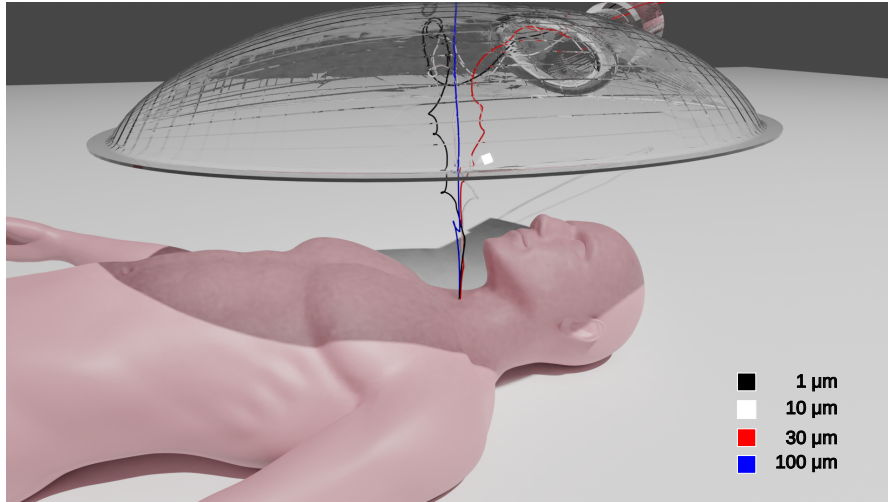


Figure 9: Some trajectories of the particles in function of the diameter

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9. Appendix

9.1. Governing equations

In this section, we describe the numerical method used to solve the Navier-Stokes equations: the high performance computational mechanics code Alya ((Vázquez et al., 2016)), which was developed at Barcelona Supercomputing Center. Let μ be the viscosity of the fluid, and ρ its constant density. The

problem is stated as follows: find the velocity $\mathbf{u}$ and mechanical pressure p in a domain Ω such that they satisfy in a time interval

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla \cdot [2\mu \varepsilon(\mathbf{u})] + \nabla p = \mathbf{o}, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2)$$

together with initial and boundary conditions. The velocity strain rate is $\varepsilon(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^t)$.

The spatially filtered Navier-Stokes equations for a fluid moving in the domain Ω bounded by $\Gamma = \partial\Omega$ during the period (t_0, t_f) repose to find a filtered velocity $\bar{\mathbf{u}}$ and a kinematic pressure p such that

$$\partial_t \bar{\mathbf{u}} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} - 2\nu \nabla \cdot \mathbf{S}(\bar{\mathbf{u}}) + \nabla p - \mathbf{f} = -\nabla \cdot \tau_{ij}(\bar{\mathbf{u}}) \quad \text{in } \Omega \times (t_0, t_f), \quad (3)$$

$$\nabla \cdot \bar{\mathbf{u}} = 0 \quad \text{in } \Omega \times (t_0, t_f), \quad (4)$$

where ν is the fluid viscosity, $\mathbf{f}$ the vector of external body forces and $\mathbf{S}(\bar{\mathbf{u}})$ is the large-scale rate-of-strain tensor. In equation (3) $\tau_{ij}(\bar{\mathbf{u}})$ is the subgrid scale (SGS) stress tensor, which must be modelled. Its deviatoric part is given by

$$\tau_{ij}(\bar{\mathbf{u}}) - \frac{1}{3} \tau_{kk}(\bar{\mathbf{u}}) \delta_{ij} = -2\nu_{sgs} \nabla \cdot \mathbf{S}(\bar{\mathbf{u}}) \quad (5)$$

where δ_{ij} is the Kronecker delta. The formulation is closed by an appropriate expression for the subgrid-scale viscosity, ν_{sgs} . In this study an eddy-viscosity subgrid-scale model (Vreman model) (Vreman, 2004) is applied. This model provided good results in previous simulations of respiratory airways (Calmet et al., 2020) or jets (Both et al., 2020) being competitive comparing with more computational demanding models like the dynamic Smagorinsky, see (Koullapis et al., 2017).

The set of equations is time integrated using an energy conserving Runge-Kutta explicit method, lately proposed by Capuano et al. (Capuano et al., 2017), combined with an eigenvalue-based time step estimator (Trias & Lehmkuhl, 2011). For more details about LES method see (Lehmkuhl et al., 2019).

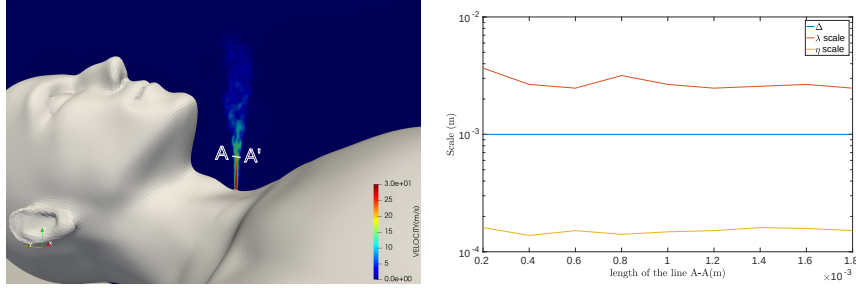


Figure 10: Comparison of different turbulence scales along the A-A' line during the jet ($t = 0.5s$ to $0.9s$), for mesh M2

9.2. Grid convergence

In the LES approach, the grid (Δ) and time resolution (Δt) are critical to ensure a reasonable ratio between the grid size and the smallest scales of turbulent motions (the Kolmogorov scale, η). While no universal criterion exist for LES grid size, a ratio $\frac{\Delta}{\eta}$ less than 20 is reasonable (Pope, 2000). The grid resolution should also fall into the turbulent length scales of the Taylor microscale (λ) and Kolmogorov scales (η). The Taylor microscale is used to characterise a turbulent flow and is larger than Kolmogorov scale (Tennekes & Lumley, 1972):

$$\lambda = \sqrt{\frac{10(\nu + \nu_{sgs})TKE}{\varepsilon}} \quad (6)$$

$$\eta = \left(\frac{(\nu + \nu_{sgs})^3}{\varepsilon} \right)^{\frac{1}{4}} \quad (7)$$

where TKE is the turbulent kinetic energy, ε is the turbulent dissipation rate, ν is the fluid kinetic viscosity, and ν_{sgs} is the subgrid-scale viscosity. Fig 10 compares the grid size (Δ) of mesh M2, with the turbulence scales during the jet ($t = 0.5s$ to $0.9s$). The profiles were taken along line A-A' which was located in the jet core at 10D of the incision. The grid size was between the Taylor and Kolmogorov scale and the equivalent ratio $\frac{\Delta}{\eta}$ was 7, which satisfied the criterion sufficient grid resolution for LES.

In addition to the turbulent length scales, the temporal resolution (Δt) is also critical to capture the highest frequencies of turbulence. The smallest time scales in a turbulent flow (the Kolmogorov time scale τ_η) is given as (Tennekes & Lumley, 1972):

$$\tau_\eta = \left(\frac{\nu + \nu_{sgs}}{\varepsilon} \right)^{\frac{1}{2}} \quad (8)$$

Based on the period ($t=0.5s$ to $0.9s$) with M2 mesh resolution along the line A-A', the minimum τ_η was equal to $6 \times 10^{-5}s$. Therefore, the time step used for the LES simulation was $1.0 \times 10^{-5}s$ (see Table 1). The time resolution of the LES simulation was sufficiently small to capture the highest frequencies of turbulence.

9.3. Particle transport and deposition modelling

Particle transport was simulated in a Lagrangian frame of reference, following each individual particle. The main assumptions of the model were:

- Particles were sufficiently small and the suspension was dilute to neglect their effect on airflow: i.e. one way coupling;
- Particles were spherical and do not interact with each other;
- Particle rotation was negligible;
- Thermophoretic forces were negligible;
- The forces considered were drag $\mathbf{F}_d$, gravitational and buoyancy $\mathbf{F}_g$;

Particles transport was predicted by solving Newton's second law, and by applying a series of forces

$$\mathbf{a}_p = (\mathbf{F}_d + \mathbf{F}_g)/m_p. \quad (9)$$

where $\mathbf{a}_p$ is the particle acceleration; m_p is particle mass, ρ_p is density, d_p is diameter, and V_p is volume.

The equation for the drag force assumed the particle reached its terminal velocity and is given by

$$\mathbf{F}_d = -\frac{\pi}{8}\mu d_p C_d \text{Re}(\mathbf{u}_p - \mathbf{u}_f), \quad (10)$$

where Re is the particle Reynolds number involving its relative velocity with the fluid:

$$\text{Re} = \frac{|\mathbf{u}_p - \mathbf{u}_f| d_p}{\nu}.$$

The drag coefficient used Ganser's formula Ganser (1993):

$$\begin{aligned} C_d &= \frac{24}{\text{Re } k_1} (1 + 0.1118(\text{Re } k_1 k_2)^{0.6567}) + 0.4305 \frac{k_2}{1 + 3305/(\text{Re } k_1 k_2)}, \\ k_1 &= \frac{3}{1 + 2\psi^{-0.5}}, \\ k_2 &= 10^{1.84148(-\log_{10}(\psi))^{0.5743}}, \\ \psi &= \text{sphericity, } (= 1 \text{ for a sphere}). \end{aligned}$$

The gravity and buoyancy forces contribute to the dynamics of the particle when there is a density difference:

$$\mathbf{b}f_g = V_p \mathbf{g}(\rho_p - \rho),$$

with $\mathbf{g}$ being the gravity vector.

Further details about particle transport and deposition modeling are available in (Calmet et al., 2018b,a).

In Order to validate the particle deposition, comparison between numerical and experimental data in the nasal cavity was used. The flow rate used for the comparison was a constant 20L/min. In order to standardize the results, the inertial parameter (IP) was used, i.e.

$$IP = d_p^2 \cdot Q \quad (11)$$

where d_a is the particle aerodynamic diameter (i.e. 1g/cm^3) and Q is the volumetric flow rate. Fig 11 shows good agreement between the simulation performed by the present code (Alya) and the numerical results of (Schroeter et al.,

2011; Shang et al., 2015; Shi et al., 2007). Differences in deposition results are due to the coarser airway surfaces in the replica producing higher deposition efficiencies than the numerical model, already observed frequently in literature, see (Shi et al., 2007; Bahmanzadeh et al., 2015) who provide an extended study which can be summarized as the “wall roughness region enhanced particle capturing effect” or other study (Ghahramani et al., 2017) who compared deposition of different level of surface roughness replicas (see Fig 11 Model A,B,C) from (Kelly et al., 2004) with LES simulations.

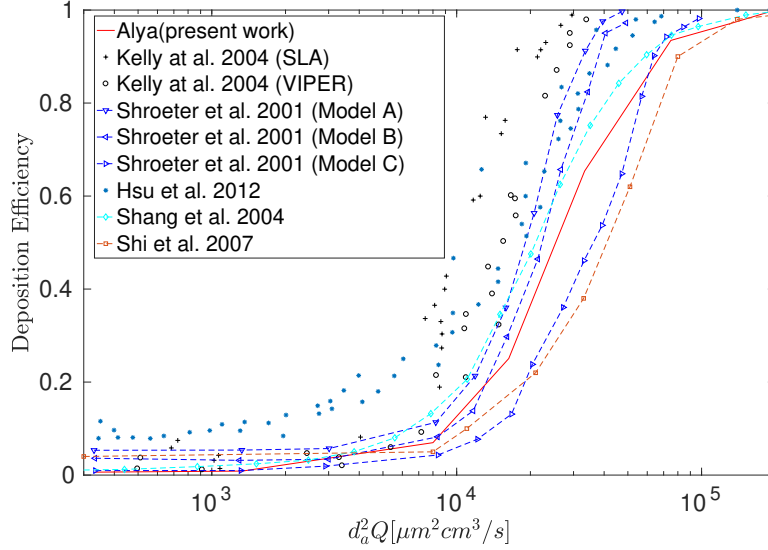


Figure 11: Micro particle deposition efficiency comparison between simulation and experiments.

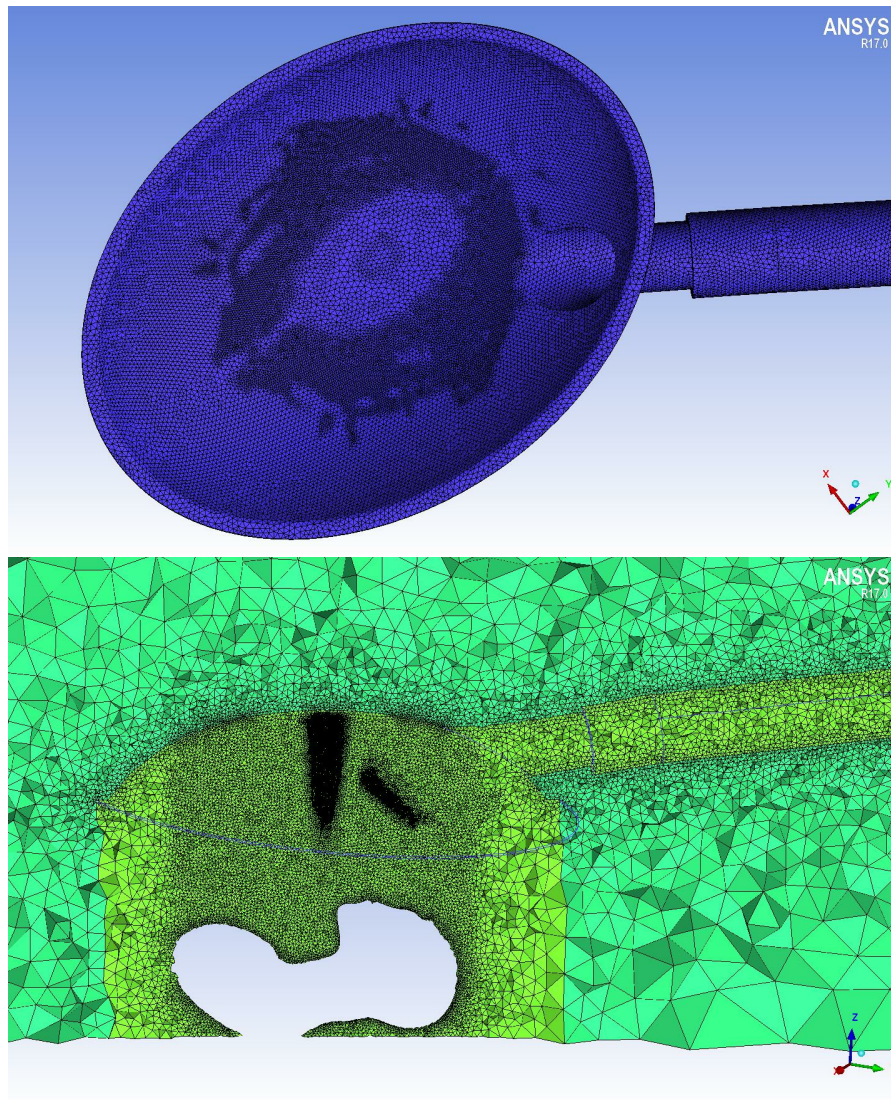


Figure 12: Detail about the mesh of the hood surface and the mesh inside of the hood